Spin-1/2 particles moving on a 2D lattice with nearest-neighbor interactions can realize an autonomous quantum computer

Dominik Janzing

Institut für Algorithmen und Kognitive Systeme,

Universität Karlsruhe, Am Fasanengarten 5, 76 131 Karlsruhe, Germany

and Institut für Quantenoptik und Quanteninformation

der Österreichischen Akademie der Wissenschaften, 6020 Innsbruck, Austria

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Abstract

What is the simplest Hamiltonian which can implement quantum computation without requiring any control operations during the computation process? In a previous paper we have constructed a 10-local finite-range interaction among qubits on a 2D lattice having this property. Here we show that pair-interactions among qutrits on a 2D lattice are sufficient, too, and can also implement an *ergodic computer* where the result can be read out from the time average state after some post-selection with high success probability.

Two of the 3 qutrit states are given by the two levels of a spin-1/2 particle located at a specific lattice site, the third state is its absence. Usual hopping terms together with an attractive force among adjacent particles induce a coupled quantum walk where the particle spins are subjected to spatially inhomogeneous interactions implementing holonomic quantum computing. The holonomic method ensures that the implemented circuit does not depend on the time needed for the walk.

Even though the implementation of the required type of spin-spin interactions is currently unclear, the model shows that quite simple Hamiltonians are powerful enough to allow for universal quantum computing in a closed physical system.

1 Introduction

To understand which sets of quantum control operations are sufficient for quantum computing is still an important issue of research. Whereas the standard model of the quantum computer is based on one- and two-qubit unitaries there is meanwhile a large number of alternative proposals, e.g. computing by measurements only [1, 2] or adiabatic computing [3, 4, 5, 6, 7]. The latter model encodes a computational problem into an interaction such that the ground state of the Hamiltonian indicates the solution. In order to understand the power of adiabatic computing it is particularly interesting to know to what extent the transition into the ground state of simple interactions can already be a non-trivial computation process. Since it has been shown that every problem in the complexity class QMA can be encoded in a nearest-neighbor interaction of qubits located on a 2D lattice [8] it is clear that, indeed, relatively simple Hamiltonians are sufficient for adiabatic computing. This highlights the computational power of simple Hamiltonians from one point of view. Another aspect of the "computational power of Hamiltonians" has been studied in models where the natural time evolution is interspersed by external control operations (see e.g. [9, 10, 11, 12]). The intention of the present paper is to understand to what extent models with simple interactions can already be autonomous devices with full quantum computing power in the sense that quantum computation reduces to the following protocol: (1) prepare an initial state in the computational basis which contains the data, (2) wait for a sufficiently long time, and (3) measure a sufficiently large set of qubits in the computational basis. In [13] we have constructed a Hamiltonian satisfying these conditions with the additional feature that the readout need not necessarily be performed within a specific time interval; in our "ergodic quantum computer" the result is also present in the time average of the dynamics after some simple post-selection with high success probability. Even though this property may be of minor practical relevance, we considered it as a necessary feature of an *autonomous* computer since one would otherwise require a clock as an additional device. Here we construct an interaction that is even simpler than the one constructed in [13] since the latter requires 10-qubit interactions.

The motivation to consider autonomous quantum computers is twofold. First, it could trigger new ideas how to reduce the set of necessary control operations in current implementation proposals by using the "natural power" of the interactions. In addressing this issue, the ergodic model defines only

an extreme case; realistic perspectives for quantum computing could arise by combining it with more conventional approaches. Second it is an interesting fundamental issue in the thermodynamics of computation how to realize computation in closed physical systems. Benioff, Feynman, and Margolus have already presented such Hamiltonian computers [14, 15, 16]. Margolus' asynchronous Hamiltonian cellular automaton (CA) has the appealing feature to be lattice-symmetric. In other words, it is driven by a finite-range interaction among qubits[1] located on a 2D lattice such that the total Hamiltonian is invariant under discrete translations. The synchronization of the CA is realized by a kind of spin wave propagating along the lattice and triggering the update of the cells according to some computationally universal update rules which are not specified any further in [16]. However, its clock wave has to start in an uncertain *position* in order to obtain a well localized *momentum* distribution with mainly positive momenta. A localized wave front would also propagate backwards and would therefore not trigger a correct computation. In [13] we have chosen the same synchronization scheme but we start with a localized wave front since we allow only for preparations of *basis* states. The fact that the dispersion of the wave front leads to completely undefined computation steps is irrelevant since the *time average* of the dynamics encodes the correct result. The feature of our ergodic model to show the correct computation result also in the time average was hence only a nice byproduct of the fact that we must use a concept which works with a strange kind of clock: The latter starts with a well-defined time but then it counts backwards and forward with completely undefined counting speed. Note that the time average can also be considered as the "generalized final state" of our computer since a final output state in the usual sense cannot exist for finite dimensional Hamiltonian models.

To ask for a simple finite range Hamiltonian that is universal for quantum computation is in some sense similar to asking for a simple computationally universal quantum cellular automaton (for some proposals see [18, 19]) with the only difference of considering update rules which change the state only in an "infinitesimal" way. However, local interactions in lattices have typically the property to spread the information into increasingly large regions, whereas it is possible to construct update rules for cellular automata that work by propagating the information forward column by column [18]. This

[1] In [17] it is furthermore argued that one of this clock Hamiltonians for CAs in one dimension is quite close to real solid state interactions.

apparent difference between discrete and continuous time dynamics can already be explained with the translation operator on n qubits: the cyclic shift is a unitary that can be achieved by local update rules [20], whereas the Hamiltonian obtained from the logarithm of the shift contains interactions between *distant* qubits. Hamiltonians with finite interaction length will typically spread the information over the lattice. Therefore, one has to be more modest and demand that the correct result can only be present with high probability.

The paper is organized as follows. In section 2 we explain the hardware of our model consisting of a chain of atoms on a 2D square lattice. We construct a nearest-neighbor interaction which leads via a simple effective Hamiltonian to a coupled random walk that will later trigger the implementation of gates acting on the atom spins. In section 3 we explain how to arrange spin-spin interactions among the atoms such that they implement logical gates based on holonomic quantum computing. In section 4 we describe the complete Hamiltonian of our computing device. In section 5 we show that the time evolution of the effective Hamiltonian is solvable since it can be transformed into a quasifree evolution of fermions. Based on this solution, we estimate the time required for the computation process. In section 6 we briefly sketch some ideas on the realization. Section 7 describes how to construct the Hamiltonian such that it implements a universal quantum cellular automaton. This is to obtain programmable hardware. In the appendix we present an alternative model for the atom propagation which is caused by an even simpler Hamiltonian since the nearest-neighbor interactions in the model presented in the main part involves also *diagonal neighbors* in the lattice. In contrast, the model in the appendix uses only *nearest* neighbors in a strict sense. However, the corresponding Hamiltonian dynamics will not be solvable. We will therefore consider an incoherent analogue and show that the corresponding classical random walk would trigger the implementation of gates in the desired way. For the coherent model, we can only conjecture that an appropriate propagation is achieved.

2 The synchronization Hamiltonian

Now we present a model of a 2D lattice with a coupled propagation of a chain of atoms which will later be the synchronization mechanism of the computer. While propagating along the horizontal direction (see Fig. 1) the

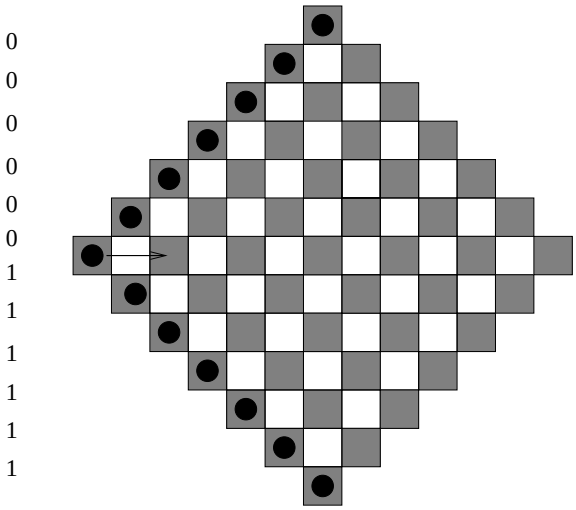

Figure 1: Initial atom configuration for a 7×7 lattice. The digits at the left indicate the corresponding binary string which will be introduced in section 5 and the arrow shows the only possible motion.

spin of the atoms (which represent the logical states) will be subjected to spatially inhomogeneous interactions that implement the desired gates. It is important that the chain does not tear since the spin-spin interactions to be described later will only be active between adjacent atoms. Furthermore, it is important for the synchronization that the chain remains connected. This will become clear in section 3.

We will now describe the synchronization Hamiltonian in detail and show that it generates a diagonalizable quantum walk. The lattice and the initial atom configuration are shown in Fig. 1. The lattice sites are given by $n \times n$ black fields of the modified chess-board in Fig. 1. The $2n-1$ atoms are only allowed to move forward or backward along the horizontal direction, i.e., along the rows. Each atom can only hop from a black site to either the next or the previous black site in the row. Furthermore, the atoms can only move such that the chain does not tear, i.e., atoms in adjacent rows are always diagonal neighbors. Fig. 2 shows a possible configuration.

Now we describe the Hamiltonian that allows only collective motions of the atoms respecting these rules. The grid of black fields is labeled by (i, j) with $i, j = 1, \ldots, n$. The sites $(1, j)$ with $j = 1, \ldots, n$ indicate the diagonal line leading from the leftmost field to the uppermost one and sites $(i, 1)$ with

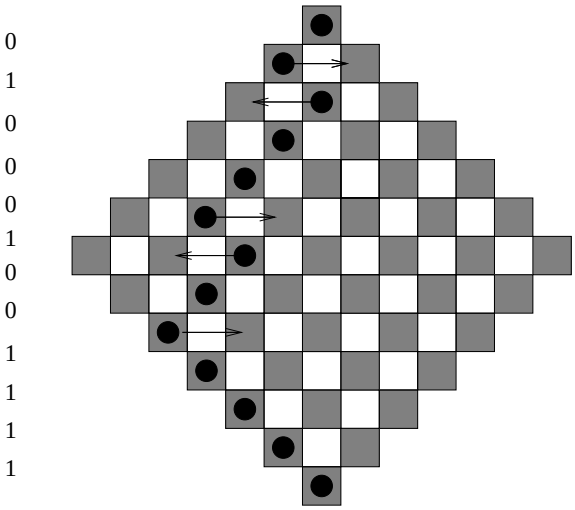

Figure 2: Possible atom configuration with its corresponding binary string (as explained in section 5) and the possible motions.

$i = 1, \ldots, n$ indicate the diagonal line from the leftmost field to the lowermost one. We consider the Hilbert space of all atom configurations as a subspace of an n^2-qubit register of the form

$$\mathcal{H}_q := (\mathbb{C}^2)^{\otimes n^2} ,$$

where qubit (i, j) corresponds to lattice site (i, j) and the basis states $|0\rangle$ and $|1\rangle$ indicate that there is no atom or that there is an atom, respectively, at position (i, j). A subspace of $\mathcal{H}_q$ is the clock Hilbert space $\mathcal{H}_c$ spanned by all *allowed* configurations. They correspond to those basis states in $\mathcal{H}_q$ for which there is exactly one atom in each row and for which the atom chain is connected. First we introduce interactions between site (i, j) and $(i+1, j+1)$ which generates independent hopping of atoms along the rows:

$$K := \sum_{i,j=1}^{n-1} \left(a_{i,j} a^\dagger_{i+1,j+1} + h.c. \right) . \tag{1}$$

To achieve that the atom configuration remains a connected chain we introduce a strong attractive force between diagonal neighbors:

$$H_{pot} := -E \sum_{<(i,j),(k,l)>} N_{i,j} N_{k,l} + E_0 \, \mathbf{1} , \tag{2}$$

where $E \in \mathbb{R}^+$ is assumed to be much larger than 1 and $N_{i,j} = a^\dagger_{i,j} a_{i,j}$ is the projection on the states with an atom in position i, j. The sum runs over all unordered pairs of sites $(i,j),(k,l)$ with $|i-k|+|j-l|=1$. The physically irrelevant term E_0 is (for purely technical reasons) chosen such that the initial configuration has zero energy. The energy is minimal if all attractive interactions are active. Otherwise, if the chain is not connected, the potential energy is at least E. We define the "synchronization Hamiltonian", which leads to the desired coupled motion of atoms, by

$$\tilde{H} := K + H_{pot}\,. \tag{3}$$

In order to analyze the dynamics generated by $\tilde{H}$ we first argue that it can be replaced with an effective clock Hamiltonian H_{eff} having $\mathcal{H}_c$ as an invariant subspace. The initial atom configuration defines a ground state of H_{pot}. Due to $E \gg 1$ the comparably small perturbation K cannot circumvent the gap to one of the first excited states of H_{pot}. If P denotes the spectral projection of H_{pot} corresponding to the ground state energy 0 we will therefore expect a dynamical evolution according to

$$H_{eff} := PKP\,. \tag{4}$$

Note that not all states in the image of P are allowed clock states since the image of P contains also states with more than one atom in a row. However, these ground states could only be reached from an allowed state if K contained hopping terms along columns.

The following lemma (proven in the appendix) justifies more formally that we may analyze the dynamics according to H_{eff} instead of $\tilde{H}$:

Lemma 1 *For $E > n^6$ and $n \geq 10$ the norm distance between the effective Hamiltonian in equation (4) and the restriction $\tilde{H}_{E/2}$ of $\tilde{H}$ to the eigenspace corresponding to eigenvalues smaller than E satisfies*

$$\|\tilde{H}_{E/2} - H_{eff}\| \leq 9\frac{n^3}{\sqrt{E}}\,.$$

If we increase the attractive part of the interaction proportional to n^6 if n increases the time evolution induced by H_{eff} is a good approximation for the true one. If the intention of this article was to propose a physical implementation scheme this would be a rather bad scaling, leading possibly

to hard practical problems. However, from the computer science point of view, it is essential that the increase of energy is only polynomial in n and we will thus obtain an *efficient* model of computation.

We will now give a more explicit form of H_{eff}. To be more precise, we will describe an operator whose restriction to $\mathcal{H}_c$ coincides with H_{eff}. Let $|c\rangle$ denote some basis state in $\mathcal{H}_c$, i.e., c describes an allowed atom configuration. Then

$$H_{eff}|c\rangle = PKP|c\rangle = PK|c\rangle = P\sum_{1=i,j}^{n-1}\Big(a_{i,j}a^{\dagger}_{i+1,j+1} + h.c.\Big)|c\rangle \qquad (5)$$

is a superposition of all atom configurations with connected chain that can be reached from c by moving one atom forward or backwards in its diagonal row. In other words, each hopping term $a_{i,j}a^{\dagger}_{i+1,j+1}$ is only active if the sites $i, j+1$ and $i+1, j$ are occupied. We have therefore a conditional hopping given by

$$H_{eff} = \sum_{i,j=1}^{n-1} a_{i,j}a^{\dagger}_{i+1,j+1}N_{i,j+1}N_{i+1,j} + h.c.\ \Big|_{\mathcal{H}_c},$$

where the symbol $\mathcal{H}_c$ at the right indicates the restriction to $\mathcal{H}_c$. Using a slightly more intuitive notation, which respects the orientation of Fig. 1, the summands of H_{eff} can be denoted by

$$\begin{array}{ccccc} & & N & & \\ & \otimes & & \otimes & \\ a & & & & a^{\dagger} \\ & \otimes & & \otimes & \\ & & N & & \end{array} \quad + \quad h.c.\,, \qquad (6)$$

where this 4-local operator acts on 4 black sites enclosing a common white site.

We are interested in the dynamical evolution of the quantum state defined by the initial atom configuration. Since it is a ground state of the dominating Hamiltonian H the major part of the state vector is contained in that spectral subspace of $\tilde{H}$ which corresponds to energy values not greater than $E/2$. Using the bound of Lemma 1 we may then estimate the error in the dynamical evolution caused by replacing the true evolution with the evolution according to H_{eff}.

Theorem 1 *Let $|\psi\rangle \in \mathcal{H}_c$ be an arbitrary allowed atom configuration. Then we have*

$$\|(e^{-i\tilde{H}t} - e^{-iH_{eff}t})|\psi\rangle\| \leq \epsilon t + 2n\sqrt{\frac{2}{E}}\,,$$

where

$$\epsilon := 9\frac{n^3}{\sqrt{E}}$$

as in Lemma 1.

Proof: Due to $H_{pot}|\psi\rangle = 0$ the average energy of $|\psi\rangle$ satisfies

$$\langle\psi|\tilde{H}|\psi\rangle = \langle\psi|K|\psi\rangle \leq \|K\| \leq n^2\,,$$

where the last inequality is given by counting the number of terms in eq. (1). Let Q be the spectral projection of $\tilde{H}$ corresponding to all eigenvalues less than E. Then we have

$$\langle\psi|Q\tilde{H}Q|\psi\rangle + \langle\psi|(\mathbf{1}-Q)\tilde{H}(\mathbf{1}-Q)|\psi\rangle = \langle\psi|\tilde{H}|\psi\rangle \leq n^2\,.$$

Using

$$\langle\psi|(\mathbf{1}-Q)\tilde{H}(\mathbf{1}-Q)|\psi\rangle \geq E\|(\mathbf{1}-Q)|\psi\rangle\|^2\,,$$

and

$$\langle\psi|Q\tilde{H}Q|\psi\rangle = \langle\psi|K|\psi\rangle \geq -\|K\| \geq -n^2$$

we conclude

$$\|(\mathbf{1}-Q)|\psi\rangle\|^2 \leq \frac{2n^2}{E}\,. \tag{7}$$

We have

$$\begin{aligned}\|(e^{-i\tilde{H}t} - e^{iH_{eff}t})|\psi\rangle\| &\leq \|(e^{-i\tilde{H}_{E/2}t} - e^{-iH_{eff}t})Q|\psi\rangle\| \\ &\quad + \|(e^{-i\tilde{H}t} - e^{-iH_{eff}t})(\mathbf{1}-Q)|\psi\rangle\| \\ &\leq \epsilon t + 2\|(\mathbf{1}-Q)|\psi\rangle\|\,, \end{aligned} \tag{8}$$

where we have used $\|\exp(iA) - \exp(iB)\| \leq \|A - B\|$ for two self-adjoint matrices A, B. The statement follows then by replacing the last term in eq. (8) with the right hand side of ineq. (7). □

One could use the condition $t \ll \sqrt{E}/(9n^3)$ of Theorem 1 to determine the time scale for which H_{eff} is a good approximation when E is given. We

can also assume that the time scale is given and we have to determine the interaction strength E. After all, we have to ensure that the approximation is valid for all $t \leq t_0$ where t_0 is some a priori given upper bound on the time required by the clock wave to pass the relevant region on the lattice, i.e., the region containing the spin-spin interactions which will be described in the next section.

The effective Hamiltonian leads to a quantum walk on the space of atom configurations which will be diagonalized in section 5. In the next section we will explain how this walk may trigger the implementation of gates.

3 Holonomic implementation of logical gates

Now we consider not only the positions of the atoms but also their inner degree of freedom, e.g. their spin. We replace the qubit at each lattice site with a qutrit and extend hence the space $\mathcal{H}_q$ to

$$\mathcal{H} := (\mathbb{C}^3)^{\otimes n^2} .$$

The basis states $|0\rangle, |\downarrow\rangle, |\uparrow\rangle$ indicate the absence of the atom or its two possible spin states, respectively. Before we describe how to add a spin-spin interaction Hamiltonian to $\tilde{H}$ which leads to the implementation of gates when the atoms are moving along the rows, we should first mention two obvious approaches to imprint gates by interactions and why they are not suitable for our goal.

In [13] and [16] the gates are directly coupled (as additional *tensor product* components) to the synchronization Hamiltonian. Certainly we could define the hopping term in eq. (1) between column j and $j+1$ in any desired row such that the spin is not conserved during the atom propagation but subjected to some rotation. This would provide us with one-qubit gates. Such a one-qubit gate would clearly be inverted when the atom moves back to column j again. The conditional state of the considered qubit, given that the atom is found on the right of column j would hence be subjected to the desired transformation, no matter whether the atom has traveled back and forth several times as is is typical for a random walk.

To imprint two-qubit gates into the Hamiltonian is more difficult. The obvious method to couple their implementation with some coupled motion of two adjacent atoms would require more non-local interactions than only two-particle terms. The second obvious method would be to complete the

clock Hamiltonian by an *additive* spin-spin interaction term between some adjacent sites in the same column. This leads to the following problems. First the atoms do not stay there for a well-defined time. Some part of the wave packet moves already and one part stays. Second the atoms travel back and forth and pass the interaction region several times. Both effects would in general entangle atom position and logical spin states in an uncontrollable way.

A solution to the latter problem is holonomic quantum computing [21, 22]. The idea of this approach, in the usual setting, is that some time-dependent Hamiltonian $G(t)$ is adiabatically changed along a closed loop such that, on an appropriate degenerate subspace, the overall effect is a unitary which depends only on the loop (described by representing $G(t)$ in some parameter space) and not on the speed of the change of $G(t)$. The unitary in the end remains the same even if the vector $G(t)$ has been moving back and forth on this loop in the parameter space.

We apply this concept to our model where we achieve the time-dependence of the spin-spin interaction by the motion of the atoms when they pass spatially inhomogeneous interactions. We imprint a spin-spin interaction (varying slowly along the rows) such that is describes a closed loop after the atoms have passed a certain region. Then the spin state of the atoms does not depend on the time required for the passing, neither does it depend on the number of times the atoms were traveling back and forth before the whole region has been passed. This ensures that the entanglement between the position degree of freedom and the spin is lost as soon as the region has been passed by the whole atom chain. Before we explain how to make use of this idea in detail, we rephrase a result in section II of Ref. [23], which is useful for us, as a lemma:

Lemma 2 (Holonomic Gates)
Given a family of Hamiltonians $G(t)$ on a finite dimensional Hilbert space $\mathcal{H}$ by

$$G(t) = e^{iXt} G_0 e^{-iXt} \quad \text{with } t \in [0, T]\,,$$

where X is a self-adjoint operator on $\mathcal{H}$ such that the family $G(t)$ is a closed loop, i.e., $G(0) = G(T)$. Let the change of $G(t)$ be sufficiently slowly to consider it as an adiabatic change, i.e., for each entry $G_{i,j}(t)$ of $G(t)$ we have

$$\left| \frac{d}{dt} G_{i,j}(t) / G_{i,j}(t) \right| \ll \Delta\,,$$

where Δ is the smallest spectral gap of $G(0)$.

Let U_T be the time evolution generated by the family $G(t)$ after the closed loop. Let $\mathcal{K}$ be an eigenspace of G_0 with eigenvalue λ. Then U_T keeps $\mathcal{K}$ invariant and its restriction is given by

$$e^{-i\lambda T} e^{iQXQT}, \tag{9}$$

where Q is the projection onto $\mathcal{K}$. The unitary (9) is also called a non-abelian geometric phase.

Since the holonomic concept implements the well defined unitary

$$\exp(iQXQT)$$

only on a *subspace* $\mathcal{K}$ of the full Hilbert space our $2n-1$ spin particles cannot be used for $2n-1$ logical qubits. Instead, the atom in row $2i-1$ will encode a logical qubit together with the atom in row $2i$. Moreover, we can only use rows being not too far from the row in the middle since the others are too short to imprint interactions that implement gates. Two adjacent spin particles encode one qubit with logical states $|0\rangle_l, |1\rangle_l$ via

$$|0\rangle_l := |\downarrow\rangle \otimes |\uparrow\rangle \quad \text{and} \quad |1\rangle_l := |\uparrow\rangle \otimes |\downarrow\rangle .$$

We will call their span $\mathcal{C}$ the "code space".

One-qubit gates

To explain how to implement one-qubit gates we first restrict our attention to two adjacent rows. We add interactions as follows. The whole region which carries the gate consists of a stripe of width 2 as shown in Fig. 3. We call this region "interaction stripe". Inside this stripe, we add a "gate Hamiltonian" to $\tilde{H}$ which consists of spin-spin interactions V_j between certain diagonal neighbors in adjacent rows (as indicated by the edges labeled with $V_1, \ldots, V_l$ in Fig. 3). Each V_j is a pair-interaction between two sites. We choose the following interactions:

$$V_j := e^{i\frac{2\pi(j-1)}{l-1}X}(\sigma_z \otimes N + N \otimes \sigma_z)e^{-i\frac{2\pi(j-1)}{l-1}X}, \tag{10}$$

with $j = 1, \ldots, l$. Here X is some self-adjoint operator on $\mathbb{C}^3 \otimes \mathbb{C}^3$ specified later and

$$N := |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\uparrow|$$

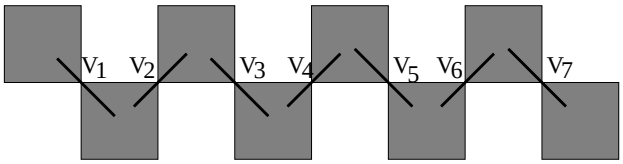

Figure 3: Spin-spin interactions for a logical one-qubit gate. Note that these are nearest neighbor interactions in a 2D lattice when the grid is oriented in diagonal direction with respect to the pattern of the chess-board.

is the particle number operator in analogy to the operator $N_{i,j}$ in eq. (2). The Pauli matrix σ_z has to be read as formally acting on the space $\mathbb{C}^3$ of the corresponding qutrit, even though it is zero for the state $|0\rangle$ and acts therefore only on the spin states. It is important to note that the degenerate eigenspace of V_0 and V_{l-1} coincides with the code space $\mathcal{C}$. If the spins are initialized such that their state is in $\mathcal{C}$ before they pass the interaction region they will at every time instant remain in the degenerate subspace of the interaction that is active (provided that the change between different V_j is adiabatic). This will implement the "non-abelian phase" $\exp(i\,QXQ\,T)$ of Lemma 2.

The length l of the interaction stripe is chosen such that the change of interactions from j to $j+1$ can be considered as approximating a continuous change and furthermore as adiabatic when the atom chain is propagating in horizontal direction. To sketch how to choose l we define a typical time scale τ on which an atom jumps from one site to its neighbor. Then we have to ensure that each entry V_j^{ik} of V_j satisfies

$$\left|\frac{V_{j+1}^{ik}-V_j^{ik}}{\tau\,V_j^{ik}}\right| \ll \Delta\,, \tag{11}$$

where Δ is the smallest energy gap of V_1. Here, the time τ is defined as a dimensionless quantity of the order 1 since the hopping terms $a_{i,j}a^\dagger_{i+1,j+1}+h.c.$ in eq. (1) appears with constant one. Physical dimensions are irrelevant since inequality (11) is invariant with respect to a simultaneous rescaling of all V_j and the hopping terms in eq. (1). We obtain therefore the dimensionless condition $l \gg 1$.

Now we may set

$$X := \sigma_x \otimes (\cos\phi\,\sigma_x + \sin\phi\,\sigma_z)\,, \tag{12}$$

with arbitrary angle ϕ, or

$$X := \sigma_y \otimes (\cos\phi\,\sigma_x + \sin\phi\,\sigma_z)\,, \tag{13}$$

where we have again slightly abused notation since we did not explicitly indicate the embedding of the 2-qubit operators in eqs. (12) and (13) (acting on the 4 possible spin configurations) into the two qutrit space. The following lemma shows which gates are implemented by the above choices for X.

Lemma 3 *Let two atoms pass a region where they are subjected to the Hamiltonians $V_1, \ldots, V_l$ in eq. (10) with X as in eq. (12) or eq. (13). Assume furthermore that l is sufficiently large to consider the change of interactions as adiabatic. Then their encoded qubit is, up to an irrelevant global phase, subjected to the transformation $\exp(2\pi\, i \cos\phi\,\sigma_x)$ or $\exp(2\pi\, i \cos\phi\,\sigma_y)$, respectively.*

Proof: On the space $\mathbb{C}^2 \otimes \mathbb{C}^2$ spanned by the 4 spin states the interaction changes according to

$$V_j := e^{i\frac{2\pi(j-1)}{l-1}X}(\sigma_z \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_z)e^{-i\frac{2\pi(j-1)}{l-1}X}\,,$$

with $j = 1, \ldots, l$. Due to Lemma 2 the code space $\mathcal{C}$ is then subjected to $\exp(i\,2\pi A)$ with $A := P_{\mathcal{C}} X P_{\mathcal{C}}$, where $P_{\mathcal{C}}$ is the projection onto $\mathcal{C}$. For both choices for X, the relevant operator A consists then only of transitions between $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, which corresponds to a σ_x if the transition amplitudes are 1 (as it is the case given by eq. (12)) and to σ_y if they are i and $-i$ (as in the case of eq. 13). □

Lemma 3 shows that we can generate arbitrary one-qubit transformations by concatenating interactions with X as in eq. (12) and (13) using appropriate angles ϕ.

Two-qubit gates

For the implementation of logical two-qubit gates we consider interaction stripes that consist of 3 adjacent rows (see Fig. 4), where row 1 and 2 belong to the *first* logical qubit and row 3 is part of the *second* logical qubit. We define interactions V and U_j such that V connects row 1 and 2 and U_j

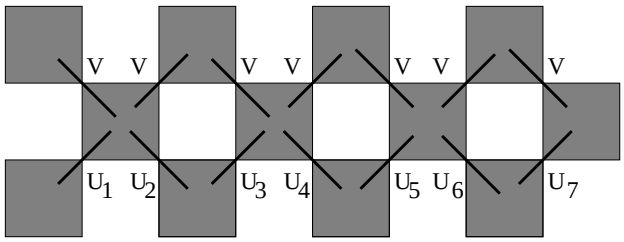

Figure 4: Spin-spin interactions for a logical two-qubit gate. Row 1 and row 2 encode one logical qubit and row 3 is part of a second qubit (together with row 4 which is not shown in the figure).

connects row 2 and 3 as shown in Fig. 4. We will refer to the atoms in row $1, 2, 3$ as atoms $1, 2, 3$, respectively.

The interaction between row 1 and the row 2 is always V in the whole interaction stripe. Row 2 interacts with row 3 according to $U_1, U_2 \ldots, U_l$.

As soon as atom 2 has entered the interaction stripe (shown in Fig. 4 for $l = 7$) it is simultaneously subjected to interactions V and U_1. Moreover, V and U_l are turned off simultaneously as soon as atom 2 leaves the interaction stripe. The total interaction that is active on the system consisting of the spins of atoms 1,2,3 is therefore either

$$V \otimes \mathbf{1} + \mathbf{1} \otimes U_j \quad \text{with } j = 1, \ldots, l\,,$$

when atom 2 is inside the interaction stripe, or 0 otherwise.

We choose

$$V := \sigma_z \otimes N\,, \tag{14}$$

where the first tensor component refers to row 1 in Fig. 4 and the second to row 2. The operator N has no effect on the spin of the atom in row 2. It only ensures that the σ_z-Hamiltonian is not switched on before the atom in row 2 has entered the left-most black field in row 3 in Fig. 4.

The interaction U_j changes according to

$$U_j := \sigma_z \otimes |\downarrow\rangle\langle\downarrow| + (e^{i\frac{2\pi(j-1)}{l-1}\tilde{X}} \sigma_z e^{-i\frac{2\pi(j-1)}{l-1}\tilde{X}}) \otimes |\uparrow\rangle\langle\uparrow|\,, \tag{15}$$

where $\tilde{X}$ is an operator that acts on the one-qutrit space. It will be specified later. On the space $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ spanned by all 8 possible spin states, we have

$$V\otimes\mathbf{1}+\mathbf{1}\otimes U_j = \sigma_z\otimes\mathbf{1}\otimes\mathbf{1}+\mathbf{1}\otimes\sigma_z\otimes|\downarrow\rangle\langle\downarrow|+\mathbf{1}\otimes(e^{i\frac{2\pi(j-1)}{l-1}\tilde{X}}\sigma_z e^{-i\frac{2\pi(j-1)}{l-1}\tilde{X}})\otimes|\uparrow\rangle\langle\uparrow|\,.$$

The idea is that the adiabatic change of the degenerate Hamiltonian on row 1 and 2 is controlled by the spin of the atom in row 3, i.e., by the logical state of the second qubit. Whenever the state in row 3 is $|\uparrow\rangle$, rows 1 and 2 are subjected to the Hamiltonians

$$\sigma_z \otimes \mathbf{1} + \mathbf{1} \otimes (e^{i\frac{2\pi(j-1)}{l-1}\tilde{X}} \sigma_z e^{-i\frac{2\pi(j-1)}{l-1}\tilde{X}}) \,,$$

otherwise they are subjected to a constant Hamiltonian. We find:

Lemma 4 *Let V and U_j be as in eq. (14) and eq. (15), respectively, such that they connect row 1 and 2 as well as 2 and 3, respectively. Choose the corresponding operator $\tilde{X}$ as*

$$\tilde{X} := cos\phi\, \sigma_x + \sin\phi\, \sigma_z \,,$$

with arbitrary angle ϕ. Consider the logical 2-qubit space $\mathcal{C} \otimes \mathcal{C}$, where the first tensor component refers to the atoms in rows 1 and 2 and the second to those in 3 and the additional row 4 (which is not depicted in Fig. 4). Then the adiabatic change of the interaction $V \otimes \mathbf{1} + \mathbf{1} \otimes U_j$ from $j = 1$ to $j = l$ implements a controlled-$\exp(i \sin\phi\, \sigma_z)$ transformation on $\mathcal{C} \otimes \mathcal{C}$ with the lower qubit as control qubit and the upper as target (in the tensor product in eq. (15) this correponds to the right and the left side, respectively).

Proof: Let the second qubit be in the logical 0 state $|0\rangle_l$. This means that the spins of atom 3 and 4 are in the state $|\downarrow\uparrow\rangle$. However, for the interaction only the state of atom 3 matters. Since it is $|\downarrow\rangle$, atoms 1 and 2 are constantly subjected to the spin Hamiltonian

$$\sigma_z \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_z \,. \tag{16}$$

Since the kernel of this operator coincides with the code space the logical state is not affected at all.

Assume now that the second qubit is in the state $|1\rangle$ and atom 3 is therefore in the state $|\uparrow\rangle$. Then atom 1 and 2 are subjected to the Hamiltonians

$$\sigma_z \otimes \mathbf{1} + \mathbf{1} \otimes (e^{i\frac{2\pi(j-1)}{l-1}\tilde{X}} \sigma_z e^{-i\frac{2\pi(j-1)}{l-1}\tilde{X}}) \,,$$

with $j = 1, \ldots, l$. Due to Lemma 2 the unitary that is implemented on the code space after such an adiabatic change is given by $\exp(i2\pi A)$ with

$$A := P_{\mathcal{C}}(\mathbf{1} \otimes X)P_{\mathcal{C}} = \sin\phi\, P_{\mathcal{C}}(\mathbf{1} \otimes \sigma_z)P_{\mathcal{C}} \,.$$

Describing this operator with respect to the logical basis $|0\rangle_l, |1\rangle_l$ we obtain the operator $\sin\phi\,\sigma_z$. This shows that the unitary $\exp(i2\pi\sin\phi\,\sigma_z)$ is implemented after the atoms have passed the interaction stripe. Since we have also shown that this unitary is only implemented if the state of the second qubit is $|1\rangle_l$, we have know shown that the net effect is a controlled-$\exp(i2\pi\sin\phi\,\sigma_z)$ gate. $\square$.

We can imprint interactions like those above between any adjacent logical qubits as well as we may obtain one-qubit rotations as in Lemma 3 by appropriate interactions. It is known that conditional phase gates together with the set of one-qubit rotations allow for universal quantum computing [24]. Hence we are able to design interactions for arbitrary quantum circuits.

4 The complete Hamiltonian

We obtain the complete Hamiltonian $\tilde{H}$ of our autonomous computing device as a sum of the synchronization Hamiltonian and the spatially inhomogeneous spin-spin interaction that implement holonomic transformations. It reads:

$$\hat{H} := H_{pot} + K + \sum_{<i,j,i',j'>} W_{i,j,i',j'}\,,$$

where H_{pot} is the strong attractive force defined in eq. 2 and K describes the hopping terms

$$K := \sum_{i,j=1}^{n-1} a_{i,j,\downarrow} a^\dagger_{i+1,j+1,\downarrow} + a_{i,j,\uparrow} a^\dagger_{i+1,j+1,\uparrow} + h.c\,,$$

where we have, in slight abuse of notation, adapted the definition of eq. (1) for spin-less creation and annihilation operators into those for spin $1/2$ particles. For instance, $a^\dagger_{i,j,\downarrow}$ creates a particle with spin down. Similarly, the term H_{pot} is adapted to spin $1/2$ particles in the sense that the particle number operator $N_{i,j}$ is given by

$$N_{i,j} = a^\dagger_{i,j,\downarrow} a_{i,j,\downarrow} + a^\dagger_{i,j,\uparrow} a_{i,j,\uparrow}\,.$$

The spin-spin interactions $W_{i,j,i',j'}$ are only non-zero if site (i,j) is adjacent to site (i',j') and if the pair of sites belongs to some interaction stripe. Inside these stripes, they are given by the interactions V, V_j, U_j described

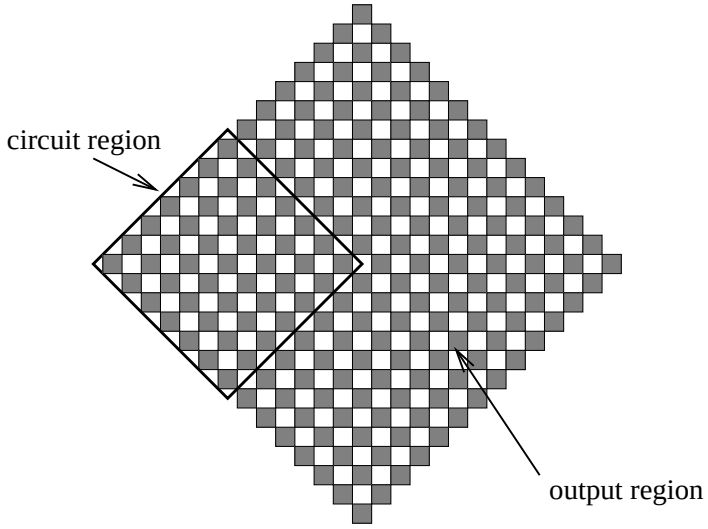

Figure 5: All spin-spin interactions implementing some circuit U are confined to the "circuit region" R. As soon as all atoms have left this region, the implementation of U is complete.

in the preceding section. We assume that all these rectangles ("interaction stripes") are confined to a square of length k, i.e., the spin-spin interaction is only non-zero for $i, j, i', j' \leq k$ for some $k < n$. We call this region the *circuit region* (see Fig. 5). As soon as all atoms have passed it, the whole circuit is implemented. The complement of the interaction region will be called *output region* since we will read out the result of the computation there.

5 Diagonalization of the quantum walk

Now we show that the Hamiltonian $\hat{H}$ leads to a propagation of atoms that implements the gates in correct order. First of all, we observe that the gates are irrelevant for the quantum walk. Different particle configurations correspond to mutually orthogonal vectors in the Hilbert space. Whether or not the particles are subjected to an additional change of their inner degree of freedom is irrelevant for the dynamics as long as we consider the adiabatic limit where the effect of the spin-spin interaction is only that it implements *unitary gates* on the spin states. Hence we will analyze the dynamics generated by H_{eff} instead of the dynamics generated by $\hat{H}$ to derive

the relevant probabilities for finding the atom chain at certain positions. After recalling that the adiabatic change of the spin-spin interactions has implemented the desired gates given that the atom chain has passed the interaction stripes we have then shown that the circuit has been implemented.

To diagonalize the quantum walk we show that it is isomorphic to a walk of free fermions propagating on a one-dimensional chain. On the left of Figs. 1 and 2 we have characterized the configurations by binary words of length $2n-2 =: 2m$. The symbols $0, 1$ as jth digit indicate whether the atom in row $j+1$ is *behind* the atom on row j or *in front* of it, respectively. The initial configuration is hence characterized by $m = n-1$ symbols 0 followed by m symbols 1. Since the atom on the very top and that one on the very bottom are fixed, the number of symbols 1 remains constant and the vector space spanned by the possible atom configurations is therefore the subspace $\mathcal{H}_m$ of $(\mathbb{C}^2)^{\otimes 2m}$ spanned by words with Hamming weight m. With respect to such a representation, the effective clock Hamiltonian H_{eff}, when restricted to $\mathcal{H}_c$, consists of operators which replace some pattern 10 by 01 or vice versa. It can be written as

$$H_s := \sum_{j=1}^{2m-1} \mathbf{1}^{\otimes j-1} \otimes |0\rangle\langle 1| \otimes |1\rangle\langle 0| \otimes \mathbf{1}^{\otimes 2m-j-1} + h.c. = \sum_{j=1}^{2m-1} b_j^\dagger b_{j+1} + h.c.\,, \quad (17)$$

where b and $b^\dagger$ are fermion annihilation and creation operators, respectively. They are defined [25, 26] by

$$b_j := \sigma_z^{\otimes j-1} \otimes |0\rangle\langle 1| \otimes \mathbf{1}^{\otimes 2m-j}\,,$$

and satisfy the canonical anti-commutation relation

$$b_i^\dagger b_j + b_j b_i^\dagger = \delta_{ij}\,\mathbf{1}\,,$$

where we have chosen the convention $\sigma_z|1\rangle = -|1\rangle$ and $\sigma_z|0\rangle = |0\rangle$.

Observe that H_s is the XY-Hamiltonian which is well-known in solid states physics [25] and generates a quasi-free evolution of fermions. Since the so-called Jordan Wigner transformation, describing the fermion interpretation formally, is standard [27], we rephrase it only briefly. The subspace $\mathcal{H}_m$ can be reinterpreted as the space of m fermions moving without interactions in a $2m$-dimensional state space. Then $\mathcal{H}_m$ is simply the antisymmetric tensor product

$$\mathcal{H}_m \equiv \underbrace{(\mathbb{C}^{2m} \otimes \cdots \otimes \mathbb{C}^{2m})^-}_{m}\,.$$

The correspondence between these two pictures can be described easily: Given a basis state in the qubit register by a binary word with symbols 1 at the positions $j_1, \ldots, j_m$. This state corresponds in the fermionic picture to

$$(|j_1\rangle \otimes |j_2\rangle \otimes \cdots \otimes |j_m\rangle)^-$$

where $|j_i\rangle$ denotes here the jth canonical basis vector in $\mathbb{C}^{2m}$.

The restriction of H_s to $\mathcal{H}_m$ is in the fermionic picture given by

$$\begin{aligned} H_s &= (S + S^\dagger) \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1} \\ &+ \mathbf{1} \otimes (S + S^\dagger) \otimes \mathbf{1} \cdots \otimes \mathbf{1} \\ &+ \ldots \\ &+ \mathbf{1} \otimes \cdots \otimes \mathbf{1} \otimes (S + S^\dagger)\,, \end{aligned}$$

where S is the linear (non-unitary) shift acting on the basis states of $\mathbb{C}^{2m}$ via

$$S|j\rangle := |j+1\rangle$$

for $j < 2m$ and $S|2m\rangle = 0$. This is because the term $\sum_j b_j^\dagger b_{j+1}$ shifts the fermion by one site. In other words, the time evolution in each tensor component in eq. (18) is generated by the Hamiltonian $S + S^\dagger$, i.e., the adjacency matrix of the linear chain. This implies that the time evolution transfers annihilators and creators to linear combinations of annihilators and creators, respectively, when considered in the Heisenberg picture [27]. Let

$$U_t := \exp(-i(S + S^\dagger)t) \tag{18}$$

be the time evolution of one particle on a quantum walk on a chain and $u_{jl;t}$ its entries. Then the time evolution of the creation operator on site j is

$$b_j^\dagger \mapsto \sum_{l \leq 2m} u_{jl;t} b_l^\dagger\,, \tag{19}$$

i.e., it evolves into an operator creating a fermion which is in a superposition of different sites. For the annihilation operator at site j we obtain

$$b_j \mapsto \sum_{l \leq 2m} \overline{u}_{jl;t} b_l\,. \tag{20}$$

To analyze the time evolution of relevant observables we will only make use of this formulation of the dynamics.

Time required for passing the circuit region

The running time of our computer is given by the length of the time one has to wait until all atoms will have passed the interaction region R, i.e., a square of length $k < n$, almost with certainty. The dynamical evolution $\exp(-iH_s t)$ is clearly quasiperiodic because the Hilbert space $\mathcal{H}_m$ is finite dimensional. Therefore the atoms will always return to R. However, the essential idea of the ergodic quantum computer is that the probability of finding it outside of R is high if one measures at a random time instant. Later, we will therefore also consider the time average, before we estimate the time needed by the atoms to pass R for the first time. We found:

Theorem 2 *Let the circuit region be a square of length k. Then there is a time $t \in O(k)$ such that the probability of finding all atoms outside the circuit region R is at least $1 - 12/k$ given that the size $n \gg k$ of the whole lattice is sufficiently large.*

The proof can be found in the appendix. Note that the probability of finding some atom in R could even be made smaller if the factor 4 in eq. (26) in the proof would be replaced with some larger number. We conclude that the implementation time for our imprinted circuit is in $O(k)$.

Computing the time average state

Now we want to show that also at a random time instant the probability of finding all atoms in the output region (i.e., the probability of finding at least k fermions on the left half) is close to 1. We found:

Theorem 3 *Let the circuit region be a square of length $k = m/4 = (n-1)/4$. Then the probability of finding all atoms outside the circuit region tends to* 1 *for $n \to \infty$.*

This theorem is also proven in the appendix. One should maybe mention the following limitation of our model: in a lattice with finite length n the adiabatic approximation underlying the holonomic implementation is only true up to some error. Therefore the implemented transformation, given that the atom chain has passed the circuit region, does not exactly coincide with the desired quantum circuit. Instead, it depends to some extent on the time needed to pass the region. In the limit of averaging the time evolution over an infinite time interval this error will increase. Roughly speaking

(and expressed in a too classical language), the atom chain has then traveled back and forth many times and the error can increase since passing the circuit region backward would not necessarily invert the implemented circuit. However, it is a matter of the time scale on which the time average is taken whether this error is relevant, i.e., the degree to which the adiabatic approximation is justified determines the time scale on which the time average is described by our analysis.

6 Remarks on the realization

To judge whether it is likely that systems with Hamiltonians as above could be found in real systems would go beyond the scope of this article. Maybe one should rather ask which modifications are possible for our models that would make them more feasible. So far, the required spin-spin interactions are quite specific.

To show that the required diagonal hopping is not a priori unphysical one could think of electrons on quantum dot arrays arranged as in Fig. 6. The hopping along the rows does not require tunneling between distant dots even though it is the *diagonal* direction with respect to the square lattice. Spin-spin interactions would then only be needed in the direction of the dashed square lattice.

Attractive interactions between particles on adjacent dots could, for instance, be achieved if the particles alternate between electrons and holes from row to row. Certainly, it will be difficult to find a system that combines the attractive interaction and the hopping with the spatially inhomogeneous spin-spin interactions.

7 Imprinting a cellular automaton

We have shown that nearest-neighbor interactions among qutrits located on a 2D square lattice can be designed in such a way that their autonomous time evolution simulates any desired quantum circuit. The Hamiltonian given here is significantly simpler than that one given in our previous paper [13] since the latter contained 10-qubit interactions. However, the advantage of the Hamiltonian in [13] is that it is programmable. The Hamiltonian given here contains the gates to be implemented already as hardware. In order to make

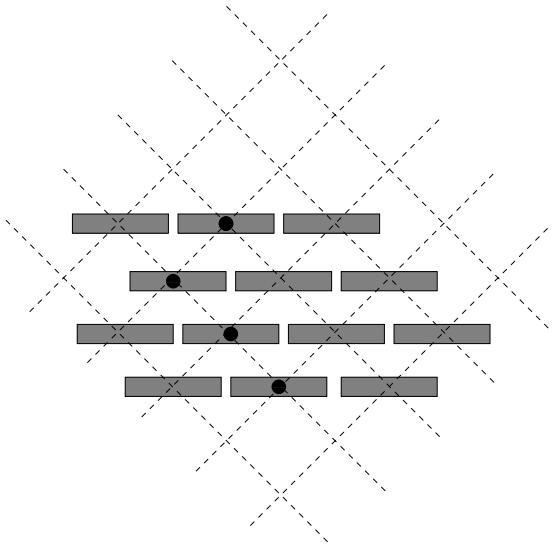

Figure 6: Schematic drawing of a dot array. The black circles indicate the particles carrying the qubits. Tunneling along the horizontal lines is possible since the distances are small. With respect to the dashed square lattice, the motion is along the diagonal direction.

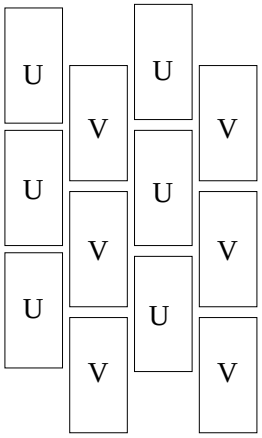

Figure 7: Interaction regions that implement a cellular automaton according to a Margolus partition scheme. A pair of columns simulates one time step of the CA.

a programmable quantum computer one could proceed as follows. Consider a universal quantum cellular automaton in one dimension [19] consisting of cells C_j with $j \in \mathbb{Z}$. Each cell contains a quantum system with Hilbert space $\mathbb{C}^d$. Using the so-called Margolus partition scheme [20, 19, 18, 16], one time step of the CA consists of two parts. The first one is given by identical copies of a unitary U acting on all pairs (C_{2j-1}, C_{2j}), the second one by identical copies[2] of V acting on all pairs (C_{2j}, C_{2j+1}). In our scheme, we may represent each cell by the subspace of an appropriate number of adjacent logical qubits. Then we cover some part of our 2D lattice with a pattern of interaction regions that implement unitaries U and V as shown in Fig. 7. The number of pairs of columns in this pattern determines the number of time steps of the simulated CA. The translation symmetry of such a crystal would then, however, be described by huge unit cells. Nevertheless, our construction shows that translation invariant finite-range interactions among finite dimensional quantum systems can in principle implement a universally programmable quantum computer.

[2]To avoid technical problems with infinite tensor products of the form $\cdots \otimes V \otimes V \otimes \cdots$ one could use a C^*-algebraic description and work with automorphisms on so-called quasilocal algebras [20].

8 Conclusions

We have shown that nearest-neighbor interactions on 2-dimensional lattices can induce dynamical evolutions that are powerful enough to represent a programmable quantum computer. Even though we have not described a realistic implementation scheme we have given interactions which are not a priori unphysical. The main reason why it may be difficult to construct systems having exactly the Hamiltonians considered here is that the spatial homogeneity of the interactions follow a rather sophisticated law.

To find even simpler Hamiltonians which can perform quantum computing in a closed physical system is an interesting challenge for further research.

Acknowledgments

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A Alternative model avoiding diagonal interactions

The clocking scheme of our autonomous computer presented so far is somewhat sophisticated in the sense that the hopping terms connect lattice sites lying diagonal with respect to the grid given by the possible atom positions. In other words, the rows defining the direction of atom propagation were *diagonal* with respect to the square lattice structure. It would be more natural to have tunneling along rows or columns of the square lattice itself.

We will therefore describe an alternative model for the propagation of an atom chain which has, however, the disadvantage, that we can only conjecture that the atoms move in forward direction with sufficient speed and will appear outside the interaction region with reasonable probability. We can, however,

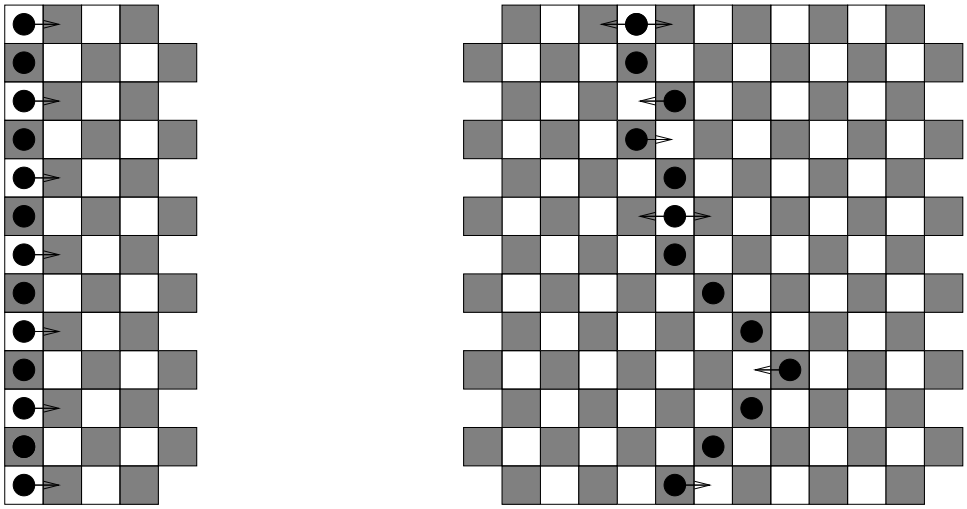

Figure 8: Left: Possible steps of atoms when they start in the first column. Right: Possible atom configuration and possible motions

prove, that the corresponding classical random walk would really implement the computation.

The whole lattice consists of $2n \times m$ sites. For reasons that will become clear later, we will color the sites such that we obtain a pattern similar to a chess board. As indicated in Fig. 8 the $2n$ atoms start in the first column. In contrast to our first model, the white sites are used, too.

The rules for the propagation of atoms along the rows are as follows. An atom on a white site is allowed to move forward or backwards by one column if the atoms in the two adjacent rows are currently in the same column. An atom on a black site is only allowed to move one column forward or backwards if it is finally located in between two adjacent atoms in the same column. In the first column, only the atoms on the white sites are allowed to move forward. A possible configuration obtained by applying these rules is shown on the left of Fig. 8.

By induction, we will argue that the configuration of atoms has always the following properties:

1. Atoms located in adjacent rows are either in the same column or in adjacent columns.

2. For every atom located on a white site there are always atoms on the

two adjacent black sites in the same column. The only exception are particles on white sites in the upper-most and lower-most rows which have certainly only one black neighbor.

It is clear that these conditions are satisfied by the initial state. In order to prove that they are preserved we observe that an atom that is located on a black site can only move to a white site if the latter is adjacent to two occupied black sites. But then it will satisfy condition (2). When an atom on a white site moves to a black site, condition (1) is certainly preserved since (2) was true for its initial position. The atoms being on black sites on the boundary can only move to column j when the atom in the row below is already in column j.

Now we present a Hamiltonian that induces these propagation rules. We start with

$$K := \sum_{k=1}^{2n} \sum_{l=1}^{m-1} a_{k,l}\, a_{k,l+1}^{\dagger} + h.c.\,,$$

which is a usual hopping term (as it appears in Hubbard models [28]) annihilating the atom at a certain position and creating it at the right or left neighboring site in the same row. Physically, one could think of an optical lattice with periodic potentials generated by standing waves which result from the superposition of counter-propagating waves [29]. To allow tunneling in horizontal direction and to avoid it along the vertical axis one could use high potential walls between rows and low potential walls between columns. This can be achieved by a superposition of high amplitude waves in vertical direction with low amplitude waves in horizontal direction.

Now we modify the lattice such that there are two types of minima in the potential. The lower potential corresponds to the black sites and the higher potential to the white sites. By superposition of two lattices with wave length λ and 2λ one could also generate a chess-board like alternating potential (this is called a "superlattice" in [30]).

We describe the alternating potential by introducing an additional term

$$H_1 := -2E \sum_{(k,l)\in B} N_{k,l}\,,$$

where B denotes the set of black sites. Furthermore we introduce an attractive interaction between atoms in adjacent rows which is only active between

pairs of atoms that are in the same column. The strength of the attractive interaction has strength E, i.e., we add a term

$$H_2 := -E \sum_{k=1}^{2n-1} \sum_{l=1}^{m} N_{k,l} N_{k+1,l} \,.$$

This ensures that all the allowed atom configurations have the same energy: when an atom sitting on a white site moves to a black one the attractive interaction is switched off, this compensates the energy gap between the black and the white site. The same is true for an atom on a black field that moves to a white field since the attractive interaction is then switched on. For the upper-most and the lower-most rows we need to decrease the energy gap between black and white sites because there is only one attractive interaction compensating it. We achieve this by adding a potential

$$H_3 := E \Big(\sum_{(1,l)\in B} N_{1,l} + \sum_{(2n,l)\in B} N_{2n,l} \Big) \,.$$

Given the Hamiltonian $H_1 + H_2 + H_3$, one checks easily that an allowed forward or backward motion of an atom leads to a configuration with the same energy. Moreover, one can see that every step of an atom that violates the propagation rules would lead to a state with different energy. We observe furthermore that forbidden motions would always lead to a configuration with higher energy and never to lower energy. This additional feature provides the scheme with some thermodynamical stability.

Now we add the small perturbation K (E is again thought to be large) to the potentials and obtain

$$\tilde{H} := H_1 + H_2 + H_3 + K \,.$$

In analogy to the discussion of our first model we obtain an effective Hamiltonian that is given by

$$H_{eff} := P \tilde{H} P \,,$$

where P is projecting onto the subspace of states having the same energy as the initial atom configuration.

The effective Hamiltonian modifies the hopping terms such that they are multiplied by an additional number operator checking the position of the atoms in adjacent rows. In other words, each term of the form $a^\dagger_{j,k} a_{j,k+1}$ as

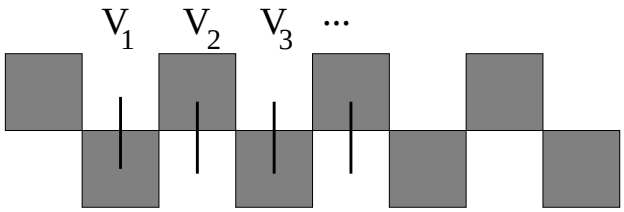

Figure 9: Spin-spin interactions for a logical one-qubit gate.

well as those of the form $a_{j,k}a^\dagger_{j,k+1}$ are only active if the two black fields are occupied which are either the current two neighbors of the considered atom (if the latter is located on a white site) or the future two neighbors (if it moves to a white site). Explicitly, we get therefore

$$\begin{array}{c} N \\ \otimes \\ a \\ \otimes \\ N \end{array} \otimes a^\dagger \quad + \quad a^\dagger \otimes \begin{array}{c} N \\ \otimes \\ a \\ \otimes \\ N \end{array} \quad + \quad h.c..$$

The operators N of these 4-local terms act on black sites in the same column.

To implement one-qubit gates in this scheme, we imprint interactions as shown in Fig. 9. The interactions $V_1, \ldots, V_l$ are chosen as in Section 3. A decisive difference to our first model is that the hopping of the atoms does not turn V_j on immediately after V_{j-1} was turned off. Instead, the atoms pass always a configuration where all interactions are turned off. However, this is irrelevant for the holonomic scheme because the statement of Lemma 2 remains certainly true if the evolution is interspersed by time intervals where $G(t)$ is completely switched off.

To implement two-qubit gates, we design the spin-spin interactions as depicted in Fig. 10. Now we have described how interactions can be imprinted that would implement the desired gates given that the whole atom chain passes indeed the circuit region.

However, as already stated, it seems to be difficult to derive explicit formulas for the dynamical evolution. We will therefore only consider the corresponding classical random walk and argue that one will have at least probability 1/2 to find all particles outside the circuit region in the time average. Here the circuit region is defined by the first k columns of the chess-board where k is chosen such that the region contains all interaction stripes. The computation result is then obtained by measuring the spin of the particles after they have left the circuit region.

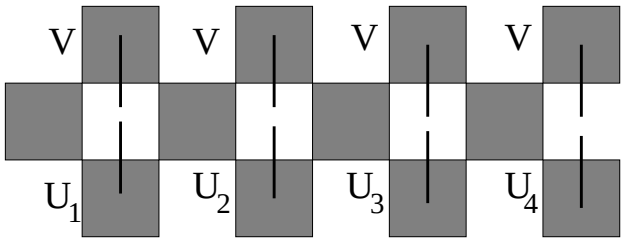

Figure 10: Spin-spin interactions for a logical two-qubit gate. Note that U_j and V are always switched on and off simultaneously since an atom can only visit a white field if the adjacent black fields in the same column are already occupied.

The classical random walk would describe the physical dynamics in the limit of strongly incoherent atom hopping. The incoherent model is, of course inconsistent with our intention to study computation in a closed physical system. The motivation to study the classical walk is that the result gives us some *small hope* that the coherent walk behaves also as it is required for computation even though it may clearly be very different from the classical random walk.

Let C be the set of allowed atom configurations on the $2n \times m$-chess-board and G be the graph with nodes C. Two nodes $c_1, c_2 \in C$ are adjacent if c_2 can be reached from c_1 by an allowed step of an atom. The probability distribution on the set of possible atom configurations at some time instant t is described by a vector $p(t) := (p_1(t), \ldots, p_l(t))$ having the l nodes of G as indices. Then a continuous classical random walk on G is described by [31]

$$\frac{d}{dt}p(t) = Lp(t)\,,$$

where L is the graph Laplacian. Its entries are $L_{ij} := -1$ for $i \neq j$ if (i, j) is adjacent, and $L_{j,j} = d_j$ where d_j is the degree of node j, i.e., its number of neighbors. Since G is connected, $\lambda_0 := 0$ is a non-degenerate eigenvalue of L [31] and there is hence a unique stationary distribution. The latter is clearly invariant if we replace each atom configuration with the configuration obtained by reflecting it at the vertical symmetry axis of the chess-board. The latter is defined by a line between column $2/m$ and $1 + 2/m$ if m, where we have assumed that m is even for simplicity.

Therefore the probability of finding at least one atom of the chain in the right half is at least $1/2$. Since the chain does not tear this implies that the

column index of every atom is at least $m/2-2n$. Provided that $k < m/2-2n$ we find with probability at least $1/2$ all atoms outside the circuit region.

B Proof of Lemma 1:

We have a dominating Hamiltonian H_{pot} and a weak perturbation K. In order to use a perturbation theorem of [8] we first have to rephrase some notations used in [8, 32].

Given a Hamiltonian H_{pot} and a small perturbation K, both acting on some finite dimensional Hilbert space $\mathcal{H}$. Let H_{pot} have a spectral gap Δ such that no eigenvalues lie between $\lambda_- = \lambda_* - \Delta/2$ and $\lambda_+ = \lambda_* + \Delta/2$ for some $\lambda_* \in \mathbb{R}$. Let $\mathcal{H}_-$ be the eigenspace of H_{pot} corresponding to the eigenvalues below λ_* and denote its complement by $\mathcal{H}_+$. Denote the corresponding spectral projections by $P_\pm$. For an arbitrary operator X, write $X_{\pm\mp}$ for $P_\pm X P_\mp$ and X_+ for $P_+ X P_+$. We define the self-energy operator $\Sigma_-(z)$ for real-valued z by

$$\Sigma_-(z) := H_{pot\,-} + K_{--} + K_{-+} G_+ (\mathbf{1} - K_{++} G_+)^{-1} K_{+-}\,,$$

where G_+, called the unperturbed Greens function (resolvent) in the physics literature, is defined by

$$G_+^{-1}(z) := z\,\mathbf{1}_+ - H_{pot\,+}\,.$$

Using the above notations, we rephrase the following theorem which can be found as Theorem 8 in [8].

Theorem 4 *Set $\tilde{H} = H_{pot} + K$ with $\|K\| \leq \Delta/2$. Let there be an effective Hamiltonian H_{eff} with spectral width w_{eff}. We assume that $H_{eff} = P_- H_{eff} P_-$. Let $0 < \epsilon < \Delta$ and furthermore*

1. *there is an $r \in \mathbb{R}$ such that*

$$w_{eff} + 2\epsilon \ll r \ll \lambda_*\,,$$

2. *for all $z \in \mathbb{C}$ such that $|z| \leq r$, $\|\Sigma_-(z) - H_{eff}\| \leq \epsilon$.*

Then the restriction $\tilde{H}_{<\lambda_*}$ of $\tilde{H}$ to the eigenspaces with eigenvalues smaller than λ_* satisfies

$$\begin{aligned} \|\tilde{H}_{<\lambda_*} - H_{eff}\| &\leq 3(w_{eff}+\epsilon)\sqrt{\frac{\|K\|}{\lambda_* + \Delta/2 - w_{eff} - \epsilon}} \\ &+ \frac{r^2\epsilon}{(r - w_{eff} - \epsilon)(r - w_{eff} - 2\epsilon)}\,. \end{aligned} \tag{21}$$

We set $\lambda_* := E/2$ and $\Delta := E$. Then the condition $\|K\| \leq \Delta/2$ is true since the expression in eq. (1) is a sum of less than n^2 terms of norm 1 and we have hence $\|K\| < n^2 < E$ due to the assumption $E \geq n^6$. For the same reason, the spectral width w_{eff} of H_{eff} is less than n^2. The operator P_- projects onto $\mathcal{H}_c$ and condition $H_{eff} = P_- H_{eff} P_-$ required by the theorem is satisfied by definition (see eq. (4)). We will now derive a bound on

$$\|\Sigma_-(z) - H_{eff}\|$$

in order to define an appropriate ϵ and a corresponding constant r.

Due to $K_{--} = P_- K P_- = H_{eff}$ and $H_{pot\,-} = 0$ we have

$$\Sigma_-(z) - H_{eff} = K_{-+} G_+ (\mathbf{1} - K_{++} G_+)^{-1} K_{+-}$$

The eigenvalues of $H_{pot\,+}$ are $E, 2E, 3E, \ldots$ according to the number of inactive interactions. Therefore the norm of

$$G_+(z) = (z\,\mathbf{1}_+ + H_{pot\,+})^{-1}$$

is at most $2/E$ for all z with $|z| \leq E/2$. With

$$(\mathbf{1} - K_{++} G_+)^{-1} = \sum_{n \geq 0} (K_{++} G_+)^n\,,$$

we have

$$\|(\mathbf{1} - K_{++} G_+)^{-1}\| \leq \sum_{n \geq 0} \Big(\frac{2\|K\|}{E}\Big)^n = \frac{1}{1 - 2\|K\|/E}\,.$$

Hence we get

$$\|\Sigma_-(z) - H_{eff}\| \leq \|K\|^2 \|G_+\| \frac{1}{1 - 2\|K\|/E}\,.$$

For $E \geq 4\|K\|$ we obtain with $\|G_+\| \leq 2/E$

$$\|\Sigma_-(z) - H_{eff}\| \leq \|K\|^2 \frac{4}{E} \leq 4\frac{n^4}{E} =: \epsilon\,.$$

We may choose $r := \sqrt{E}$ in order to fulfill $w_{eff} + 2\epsilon \ll r \ll \lambda_*$. We may now use inequality (21) and obtain

$$\begin{aligned} \|\tilde{H}_{E/2} - H_{eff}\| &\leq 3(n^2+1)\sqrt{\frac{n^2}{E-n^2-1}} \\ &+ \frac{4n^4}{(\sqrt{E}-n^2-1)(\sqrt{E}-n^2-2)}\,, \end{aligned}$$

where we have inserted the following results and definitions from above: $w_{eff} < n^2$, $\lambda_* = E/2$, $\Delta = E$, $r = \sqrt{E}$. We have inserted $\epsilon = 4n^4/E$ only in the numerator of the second fraction and replaced it with 1 (as an upper bound) at the other places. Using $E - n^2 - 1 > E/2$ for $E > n^6$ and $n \geq 10$ and $\sqrt{E} - n^2 - 2 > \sqrt{E}/2$ we have

$$\|\tilde{H}_{E/2} - H_{eff}\| \leq 4n^2\sqrt{\frac{2n^2}{E}} + \frac{16n^4}{E} \leq 9\frac{n^3}{\sqrt{E}}\,,$$

where we have used $16n^4/E < n^6/E < n^3/\sqrt{E}$. Thus, we have obtained the desired upper bound on the norm distance between $\tilde{H}_{E/2}$ and H_{eff}.

C Proof of Theorem 2

Let

$$|I\rangle := |0\ldots01\ldots1\rangle \in \mathcal{H}_m \tag{22}$$

be the initial configuration when denoted in the qubit picture. Recall the beginning of section 5, where we have described the correspondence between clock states and binary words (as indicated by the sequence of symbols 1 and 0 at the left of Figure 1).

Then all atoms are outside of R if and only if at least k symbols 1 have traveled from the right half of the chain to the left half, i.e., at least k fermions are contained in the left half of the interval of length $2m$. We have therefore to solve a mixing problem of a "discrete free fermion gas" where all particles start in the right interval. First we show that after the time $O(k)$

it is likely that at least k symbols 1 can be found on the left side. We define the observable

$$\mathcal{N} := \sum_{j=1}^{m} P_j \,,$$

where $P_j := b_j^\dagger b_j$ is the projector on the upper state of qubit j. The observable $\mathcal{N}$ counts the number of symbols 1 on the left side. In Figure 2 this corresponds to the number of symbols 1 above the row in the middle. We will estimate the probability that less than k symbols 1 have moved to the left by the Chebyshev inequality. It states that for any random variable X we have

$$P(|X - E(X)| \geq \epsilon) \leq \frac{V(X)}{\epsilon^2} \,, \tag{23}$$

where $E(X)$ and $V(X)$ denote the expectation value and the variance of X, respectively. In the sequel we will consider the probability distribution of $\mathcal{N}$ as the distribution of such a classical random variable.

Let $|I_t\rangle$ be the time evolved state after time t. Then the expectation value of $\mathcal{N}$ after the time t is given by

$$E_t(\mathcal{N}) := \sum_{j=1}^{m} \langle I_t | P_j | I_t \rangle = \sum_{j=1}^{m} \langle I_t | b_j^\dagger b_j | I_t \rangle \,. \tag{24}$$

Using the dynamics (19) and (20) we get

$$\begin{aligned} \langle I_t | P_j | I_t \rangle &= \langle I_t | b_j^\dagger b_j | I_t \rangle = \sum_{l=1}^{2m} u_{jl;t}\, \overline{u}_{jl;t} \langle I | b_l^\dagger b_l | I \rangle \\ &= \sum_{l=m+1}^{2m} u_{jl;t}\, \overline{u}_{jl;t} = \sum_{l=m+1}^{2m} |u_{jl;t}|^2 \,, \end{aligned} \tag{25}$$

where we have used that $\langle I | b_l^\dagger b_l | I \rangle$ is 1 or 0 depending on whether there the state $|I\rangle$ contains the symbol 1 at this position. Each term $|u_{jl;t}|^2$ is the probability for a particle starting at site l to be found at site j when measured after the time t in a single particle quantum walk on a linear chain of length $2m$. Since the time evolution of such a walk has been discussed in detail in the literature [33], we will only describe the implications for our model.

Consider a particle starting at site l with

$$m+1 \leq l \leq m+4k\,. \tag{26}$$

In the notation of eq. (22) such a fermion corresponds to one of the $4k$ leftmost symbols 1. The assumption $n \gg 4k$ and hence $m \gg 4k$ ensures that the time interval considered in the sequel is sufficiently small compared to the time to reach the boundaries of the lattice. Then reflections at the boundaries can be neglected. We have to wait only the time $O(k)$ in order to achieve that the width of the wave function of a particle starting at a definite position is much larger than $4k$ (see [33]) but still smaller than the size n of the whole computer. Then the probability of finding it on the left half is larger than 1/3. Recalling that this holds true for each l satisfying eq. (26) and that the number of expected fermions ($\equiv$ symbols "1") in the left half is given by the sum in eq. (24), we may choose a time instant $t \in O(k)$ such that the expectation value satisfies exactly

$$E_t(\mathcal{N}) = \frac{4}{3}\; k\,.$$

In order to estimate the variance

$$V_t(\mathcal{N}) = E_t(\mathcal{N}^2) - (E_t(\mathcal{N}))^2\,, \tag{27}$$

we observe that eq. (24) implies

$$(E_t(\mathcal{N}))^2 = \sum_{i,j\leq m} \langle I_t|P_i|I_t\rangle\langle I_t|P_j|I_t\rangle\,. \tag{28}$$

Moreover, we have

$$E_t(\mathcal{N}^2) = \sum_{i,j\leq m} \langle I_t|P_iP_j|I_t\rangle = \sum_{i,j\leq m, i\neq j} \langle I_t|P_iP_j|I_t\rangle + E_t(\mathcal{N})\,, \tag{29}$$

where we have used

$$\sum_{i=1}^{m}\langle I_t|P_iP_i|I_t\rangle = \sum_{i=1}^{m}\langle I_t|P_i|I_t\rangle = E_t(\mathcal{N})\,,$$

due to eq. (24). We rewrite one summand of the first term on the right of eq. (29) as

$$\langle I_t|P_iP_j|I_t\rangle = \sum_{l,s,r,p=1}^{2m} u_{il;t}\,\overline{u}_{is;t}\,u_{jr;t}\,\overline{u}_{jp;t}\langle I|b_l^\dagger b_s b_r^\dagger b_p|I\rangle\,. \tag{30}$$

The inner product can only be nonzero if annihilators meet creators, i.e., if either $l = s$ and $r = p$ or $l = p$ and $s = r$ or if all indices coincide. In the first case (including the third) the term is only non-vanishing for $l = s > m$ and $r = p > m$ since $b_l^\dagger b_l$ is the projection $|1\rangle\langle 1|$ on qubit l. In the second case we must have $l = p > m$ and $s = r \leq m$ since $b_s b_s^\dagger$ is the projection $|0\rangle\langle 0|$ on qubit s. Hence eq. (30) becomes

$$\sum_{m<l,\, s\leq 2m} u_{il;t}\, \overline{u}_{il;t}\, u_{js;t}\, \overline{u}_{js;t} + \sum_{m<l\leq 2m,\, s\leq m} u_{il;t}\, \overline{u}_{jl;t}\, u_{js;t}\, \overline{u}_{is;t}\,. \tag{31}$$

The first term coincides with $\langle I_t|P_i|I_t\rangle\langle I_t|P_j|I_t\rangle$ by eq. (25). We rewrite the second term as

$$\begin{aligned} & \sum_{m\leq l\leq 2m, s\leq m} u_{il;t}\, \overline{u}_{jl;t}\, u_{js;t}\, \overline{u}_{is;t} \\ = & \sum_{1\leq l\leq 2m,\, s\leq m} u_{il;t}\, \overline{u}_{jl;t}\, u_{js;t}\, \overline{u}_{is} - \sum_{1\leq l\leq m} u_{il;t}\, \overline{u}_{jl;t} \sum_{1\leq s\leq m} u_{js;t}\, \overline{u}_{is;t} \\ = & -|\sum_{1\leq l\leq m} u_{il;t}\, \overline{u}_{jl;t}|^2\,, \end{aligned}$$

where the last equality is due to

$$\sum_{1\leq l\leq 2m} u_{il;t}\overline{u}_{jl;t} = \delta_{ij}\,,$$

because U_t is unitary (see eq. 18). Hence we have found

$$\langle I_t|P_iP_j|I_t\rangle \leq \langle I_t|P_i|I_t\rangle\langle I_t|P_j|I_t\rangle \quad \forall i \neq j\,. \tag{32}$$

Combining (27) and (32) with (28) straightforward computation shows

$$V_t(\mathcal{N}) \leq \Big(E_t(\mathcal{N}) - \sum_{i\leq m}(\langle I_t|P_i|I_t\rangle)^2\Big) \leq E_t(\mathcal{N})\,. \tag{33}$$

Recall that we have chosen the time instant such that $E_t(\mathcal{N}) = 4k/3$ and hence $V_t(\mathcal{N}) \leq 4k/3$ by ineq. (33). Assume we would find less than k symbols 1 on the left half. Then the random variable defined by $\mathcal{N}$-measurements would deviate at least $k/3$ from its expectation value. Hence we can apply eq. (23) with $V_t(\mathcal{N}) \leq 4k/3$ and $\epsilon^2 = k^2/9$ and find that the probability of finding less than k symbols in the left half is at most $12/k$. This completes the proof.

D Proof of Theorem 3

In analogy to the proof of Theorem 2 we will compute the expectation value and the variance of $\mathcal{N}$ in the time average state and then use the Chebyshev inequality (23).

The time average expectation value of the fermion number on the left half is given by averaging eq. (24) over all t:

$$E(\mathcal{N}) := \lim_{T\to\infty} \frac{1}{T}\int_0^T E_t(\mathcal{N})\, dt = \sum_{l=m+1}^{2m} \Big(\sum_{j=1}^{m} \lim_{T\to\infty} \frac{1}{T}\int_0^T |u_{jl;t}|^2\, dt \Big)\,, \quad (34)$$

where the last equality follows from eq. (25). Recall that we interpret each summand for $l = m+1, \ldots, 2m$ as the probability of finding a particle (that has started at site l) in the left half of the chain when measured at a random time instant. We will show that it is close to $1/2$ up to an error in $O(1/\sqrt{m})$. It is known [34] that the Hamiltonian $S+S^\dagger$ on $\mathbb{C}^{2m}$ generating the walk (i.e., the adjacency matrix of the "path graph P_{2m}") has $2m$ different eigenvalues

$$\lambda_r = 2\cos\frac{r\pi}{2m+1} \quad r = 1, \ldots, 2m\,.$$

The eigenspaces of $S+S^\dagger$, are therefore one-dimensional and the rth eigenvector is given by [35]

$$|e_r\rangle := \sqrt{c}\sum_{j=1}^{2m} \cos\Big((j-\frac{1}{2})(r-1)\frac{\pi}{2m}\Big)|j\rangle\,,$$

where the normalization factor is $c = 1/(2m)$ for $r = 1$ and $c = 1/m$ for $r \neq 1$.

Using these eigenvectors, we may write the time average density matrix of a particle that has started at position l as

$$\sum_{r=1}^{2m} |e_r\rangle\langle e_r|l\rangle\langle l|e_r\rangle\langle e_r|\,.$$

By evaluating the probability to be at position j using this state we may compute the time average in eq. (34) and obtain

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |u_{jl;t}|^2\, dt = \sum_{r=1}^{2m} |\langle j|e_r\rangle|^2\, |\langle e_r|l\rangle|^2\,. \quad (35)$$

Each eigenvector defines a probability distribution p_r on $\{1,\ldots,2m\}$ by

$$p_r(j) := |\langle j|e_r\rangle|^2 = \frac{c}{2}\Big[1+\cos\Big((j-\frac{1}{2})(r-1)\frac{\pi}{m}\Big)\Big]\,. \tag{36}$$

The spatial probability oscillations are given by waves with frequencies $\nu_r := (r-1)\pi/m$. We will refer to those frequencies ν that satisfy

$$2\pi\frac{1}{\sqrt{m}} \leq \nu \leq 2\pi(1-\frac{1}{\sqrt{m}})$$

as *high* frequencies (they are neither close to 0 nor close to 2π) and to the others as *low* frequencies. For a high frequency wave, the probability distribution $j \mapsto p_r(j)$ leads almost to equal probabilities for both halfs. This is seen from

$$\sum_{j=1}^{m} p_r(j) = \frac{1}{2} + \frac{1}{m}\sum_{j=1}^{m}\cos(j\nu_r - \frac{\nu_r}{2})\,.$$

The sum over the oscillating terms can be bounded from above by observing

$$|\sum_{1\leq l\leq m}\cos(l\nu-\frac{\nu}{2})| \leq |\sum_{1\leq l\leq m} e^{il\nu}| \leq \frac{2}{|1-e^{i\nu}|} \in O(\sqrt{m})\,,$$

where we have used that ν differs from both 0 and 2π by $\Omega(1/\sqrt{m})$ and the last inequality follows directly from the geometric sum formula

$$\sum_{j=0}^{n} q^j = \frac{1+q^{n+1}}{1-q}\,.$$

Using eq. (35) and eq. (36), the term in the bracket in eq. (34) can be written as

$$\sum_{j=1}^{m}\sum_{r=1}^{2m} p_r(j)\,|\langle e_r|l\rangle|^2\,. \tag{37}$$

Neglecting the low frequency terms p_r in this sum can only cause an error in $O(1/\sqrt{m})$ due to $|\langle e_r|j\rangle|^2 \in O(1/m)$ taking into account that there are $O(\sqrt{m})$ such terms. Hence the probability of finding a particle that has started at any site l in the left half is close to $1/2$ up to an error in $O(1/\sqrt{m})$. By summation over all $l = m+1,\ldots,2m$ we find $E(\mathcal{N}) - m/2 \in O(m/\sqrt{m})$.

To derive bounds on the variance of $\mathcal{N}$ in the time average state we use eq. (29) and observe

$$E(\mathcal{N}^2) = \sum_{1\leq i,j\leq m, i\neq j} \text{average}\Big(\langle I_t|P_iP_j|I_t\rangle\Big) + E(\mathcal{N}) \tag{38}$$

$$\leq \sum_{1\leq i,j\leq m, i\neq j} \text{average}\Big(\langle I_t|P_i|I_t\rangle\langle I_t|P_j|I_t\rangle\Big) + E(\mathcal{N})\,, \tag{39}$$

where the last inequality is due to ineq. (32). We may rewrite the term in the big bracket in equation (39) using eq. (25) into

$$\langle I_t|P_i|I_t\rangle\langle I_t|P_jI_t\rangle = \sum_{l=m+1}^{2m} |u_{il;t}|^2 \sum_{l=m+1}^{2m} |u_{jl;t}|^2\,. \tag{40}$$

Recall that the coefficients $u_{il;t}$ are the matrix entries of a unitary that describes a random walk on a linear chain. Note furthermore that the corresponding unitary group U_t is generated by a real-symmetric Hamiltonian and we have therefore $u_{il;t} = u_{li:t}$. Thus, we are allowed to interpret $|u_{il:t}|^2$ as the probability for finding a particle at position l that has started at position i, which interchanges the original roles of i and l. This will be convenient in the sequel. The product of the sums on the right hand side of eq. (40) can either be interpreted as arising from two independent walks of two particles or the walk of one particle in two dimensions. Explicitly, we consider a dynamical evolution in $\mathbb{C}^{2m}\otimes\mathbb{C}^{2m}$ generated by the Hamiltonian

$$(S+S^\dagger)\otimes\mathbf{1} + \mathbf{1}\otimes(S+S^\dagger)\,. \tag{41}$$

Since the Hamiltonian (41) is the adjacency graph of the square lattice

$$\{1,\ldots,2m\}\times\{1,\ldots,2m\}\,,$$

we can consider the right hand of eq. (40) as the probability of finding a particle starting at $|i,j\rangle$ in a quantum walk on the square lattice in the "target quadrant" $\{m,\ldots,2m\}\times\{m,\ldots,2m\}$. We want to prove that we have sufficient mixing in order to obtain $1/4$ for the time average of term (40) up to an error in $O(1/\sqrt{m})$. We proceed similarly as for the one-dimensional walk with the essential difference that the spectrum of the Hamiltonian (41) is degenerate since $|e_r,e_p\rangle := |e_r\rangle\otimes|e_p\rangle$ and $|e_p,e_r\rangle$ have the same eigenvalues. We denote the projection onto their span by $P_{r,p}$. The rank of $P_{r,p}$ is 2 for

$r \neq p$ and 1 for $r = p$. Using these projections, we may compute the time average of (40) for fixed i, j by

$$\sum_{l,s=m+1}^{2m} \sum_{r,p=1}^{2m} \langle l, s|P_{r,p}|i, j\rangle\langle i, j|P_{r,p}|l, s\rangle = \sum_{l,s=n+1}^{2m} \sum_{r,p=1}^{2m} q_{r,p}(l, s)\, d_{r,p}\,, \qquad (42)$$

where we have defined the coefficients

$$d_{r,p} := \sum_{l,s=1}^{2m} |\langle l, s|P_{r,p}|i, j\rangle|^2 = \langle i, j|P_{r,p}|i, j\rangle$$

and probability measures $q_{r,p}$ on the square lattice by

$$q_{r,p}(l, s) := \frac{1}{d_{r,p}} |\langle l, s|P_{r,p}|i, j\rangle|^2\,.$$

Defining the frequencies $\nu_r := (r-1)\pi/n$ and $\nu_p := (p-1)\pi/n$, the state vector given by normalizing $P_{r,p}|i, j\rangle$ for a given r, p is a superposition of cosine wave functions with frequency vector (ν_r, ν_p) with another wave having the vector (ν_p, ν_r). The corresponding probability distributions $q_{r,p}$ contains then terms with frequencies $2\nu_r, 2\nu_p, \nu_r - \nu_p, \nu_r + \nu_p$. We refer to a term as low frequency term whenever at least one of these frequencies is low. For each "high frequency distribution" $q_{r,p}$ the probability for the target quadrant is $1/4$ up to an error in $O(1/\sqrt{m})$. This is seen in straightforward analogy to the corresponding argument for the one-dimensional walk. Moreover, the contribution of the low frequency terms in (42) can be bounded from above by the number of low frequency terms (which is in $O(m\sqrt{m})$) times the maximal coefficient $d_{l,s}$ of each term (which is in $O(1/m^2)$ due to $|\langle i, j|e_r, e_p\rangle| \in O(1/m)$). We conclude that the total contribution of all low frequency terms to (42) is in $O(1/\sqrt{m})$. Hence the total sum in eq. (42) is $1/4$ up to an error in $O(1/\sqrt{m})$. We conclude

$$\sum_{1\leq i,j\leq m, i\neq j} \text{average}\Big(\langle I_t|P_i|I_t\rangle\langle I_t|P_j|I_t\rangle\Big) = \frac{m^2}{4} + O(m/\sqrt{m})\,.$$

Using eq. (39) we conclude

$$E(\mathcal{N}^2) = m^2/4 + E(\mathcal{N}) + O(m/\sqrt{m})$$

and hence

$$E(\mathcal{N}^2) = (E(\mathcal{N}))^2 + O(m)\,.$$

Hence the variance $E(\mathcal{N}^2) - (E(\mathcal{N}))^2$ is in $O(m)$ and the probability that a measurement of $\mathcal{N}$ leads to a result with less than $m/4$ converges to zero with $O(1/m)$ by the Chebyshev inequality. Therefore, the probability of finding less than $m/4$ fermions on the left half (i.e., the atom chain has left the circuit region) tends to zero, too.

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